Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-

13516-27-3 | DTXSID7042015

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.84e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.66e-01

Confidence level: 3.71e-01

Nearest Neighbors from the Training Set

Image not found
Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-
Measured: 2.15
Predicted: 9.84e-01

Image not found
Dodine
Measured: 2.77e-03
Predicted: 2.87e-03

Image not found
Dodine
Measured: 2.19e-03
Predicted: 2.87e-03

Image not found
1,3-Diphenylguanidine
Measured: 4.73e-03
Predicted: 2.00e-03

Image not found
Aziprotryne
Measured: 2.44e-04
Predicted: 1.08e-02